Universal Asymptotic Eigenvalue Distribution of Density Matrices and Corner Transfer Matrices in the Thermodynamic Limit

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(February 1, 2008)

We study the asymptotic behavior of the eigenvalue distribution of the corner transfer matrix (CTM) and the density matrix (DM) in the density-matrix renormalization group. We utilize the relationship DM = CTM^4 which holds for non-critical systems in the thermodynamic limit. We derive the exact and universal asymptotic form of the DM eigenvalue distribution for a class of integrable models in the massive regime. For non-integrable models, the universal asymptotic form is also verified by numerical renormalization group calculations.

PACS numbers: 05.50.+q, 05.20.-y, 75.10.Jm, 11.30.-j

The density matrix renormalization group (DMRG) invented by S.R. White [1] is one of the most important numerical methods developed recently. Due to the remarkable success, the method has now become one of the standard methods for studying one-dimensional (1D) quantum systems [2] and two-dimensional (2D) classical statistical systems. [3] In spite of the success, little has been understood as for the foundation of the method. Studies clarifying the "origin" of efficiency of the method are important because they lead to various (including higher-dimensional [4]) extension of the method. One example is the work of Ref. [5], where a relationship between the density matrix (DM) and Baxter's corner transfer matrix (CTM) [7–9]is pointed out and a new algorithm (CTMRG) is devised. Another example is the work of Ref. [10], where it is pointed out that the DMRG (at its thermodynamic limit) is a variational method using the matrix-product-ansatz (MPA) wavefuntion as a trial wavefunction. This leads to a direct variational method which does not need the DM [10], and the product-wavefunction RG (PWFRG) which fully utilizes the MPA form of the DMRG-fixed-point wavefunction. [6]

The central object in the DMRG is the DM which is made from the groundstate wavefunction (resp. maximal eigenvalue wavefunction) of quantum Hamiltonian (resp. transfer matrix) by tracing out information of one half of the system. Keeping up to a cut-off-eigenvalue eigenstate of the DM, we have a truncated basis set consisting of a finite number (conventionally denoted by "m") of bases, to describe the remaining half of the system.

Since the accuracy of the DMRG is determined by the cut-off eigenvalue, it is crucially important to investigate the eigenvalue spectrum $\{\omega_m\}$, in particular, its asymptotic ($m \to \infty$) behavior which has not been known precisely. In this Letter, we present the *exact asymptotic form* of the DM eigenvalue distribution for a class of (non-critical) integrable models, and further, make the first systematic study for non-integrable systems employing the CTMRG and the PWFRG by which we can efficiently obtain the "fixed-point" (thermodynamic limit of the system) of the DMRG.

Let us first discuss the integrable cases. In these cases, 1D quantum problems are equivalent to 2D classical statistical problems: the Hamiltonian of the former can be derived by a log-derivative of the transfer matrix of the latter, and the ground-state wavefunction of the former is identical to the maximal-eigenvalue eigenfunction $\Psi_{\max}$ of the latter. [9] Hence, we discuss only 2D classical cases in the below.

As has been pointed out by Baxter, [9] the wavefunction (WF) $\Psi_{\max}$ is interpreted as a product of two CTMs, in the thermodynamic limit. Since the DM is just a square $\Psi^2_{\max}$ (with $\Psi_{\max}$ being regarded as a "wavefuntion matrix"), this interpretation leads to a relationship [5] between the DM, the WF and the CTM for 2D classical systems (at least non-critical case where the boundary effect is negligible), which is symbolically written as

$$\begin{aligned} \mathrm{WF} &= (\mathrm{CTM})^2, \\ \mathrm{DM} &= (\mathrm{CTM})^4. \end{aligned} \tag{1}$$

For integrable models, diagonal form of the CTM is easily known, from which we can obtain, for example, the exact one-point function (spontaneous magnetization, etc). [9] Due to the relationship (1), the diagonal form is also useful to obtain the exact eigenvalue spectrum of the DM.

We discuss the simplest case where the diagonal form of the CTM is given by a single infinite tensor product; [9] due to (1), diagonal form of the DM has the same infinite-tensor-product form with redefined parameter. For definiteness let us consider two cases (Type I and Type II) where the exact diagonal form of the DM is given by

$$\rho^{(\mathrm{diag})} = \bigotimes_{n=1}^{\infty} \begin{pmatrix} 1 & 0 \\ 0 & z^{c_n} \end{pmatrix} \tag{2}$$

with $c_n = n$ for Type I models (e.g, transverse-field Ising chain, 6-vertex model, eight-vertex model, XXZ-chain and XYZ-chain) and $c_n = 2n - 1$ for Type II models

(e.g., the square-lattice Ising model in the conventional (not eight-vertex) representation). [9] The parameter z ($0 < z < 1$) represents "degree of non-criticality" (i.e., $z \to 1$, on approaching the critical point), and how it relates to "physical" parameters depends on the model. Note that the DM (2) is unnormalized. It is "normalized" in such a way that its maximal eigenvalue ω_0 is unity; we should divide it by $\mathrm{Tr}\rho^{(\mathrm{diag})}$ for conventional normalization.

Due to the tensor-product structure (2), each eigenvalue of $\rho^{(\mathrm{diag})}$ has the form z^n with n (≥ 0) being an integer. Further, each eigenvalue z^n may have degeneracy $p(n)$. To study the degeneracy structure of the DM, it is convenient to consider $\mathrm{Tr}\rho^{\mathrm{diag}}$:

$$\mathrm{Tr}\rho^{\mathrm{diag}} = \prod_{n=1}^{\infty}(1+z^{c_n}) = \sum_{n=0}^{\infty} p(n) z^n, \tag{3}$$

where the degeneracy $p(n)$ is precisely the coefficient of z^n in the infinite series. We should note that, taking the degeneracy into account, the number of retained bases m in the DMRG should be

$$m = m(n) = \sum_{k=0}^{n} p(k), \tag{4}$$

which means that the cut-off eigenvalue of (unnormalized) DM is z^n and that we should retain all the degenerate bases belonging to this cut-off eigenvalue.

Our problem is to obtain the large-n behavior of $m = m(n)$. For this purpose, we should know the asymptotic behavior of $p(n)$. The partition theory of integers, which has been played an important role for studies of integrable IRF (interaction-round-a-face) models, is helpful again. [11] By $r(n)$ we denote the number of partitions of a positive integer n under a restriction "r" Consider the generating function $f(q)$ associated with the restricted partition problem. It has been known [11] that for a wide class of partition problems, $f(q)$ can also be given in an infinite-product form:

$$f(q) \equiv \sum_{n=0}^{\infty} r(n) q^n = \prod_{n=0}^{\infty}(1-q^n)^{-a_n} \tag{5}$$

where each a_n is a non-negative real number. For the Type I case, we have $a_n = 1$ for n odd, and $a_n = 0$ otherwise.

The asymptotics of the generating function of the form (5) is calculated by the saddle point method; $r(n)$ for $n \gg 1$ is then given by Meinardus's theorem (cited in Ref. [11], page 89):

$$r(n) = An^{\kappa}\exp(Bn^{\alpha/(1+\alpha)}) + (\text{less dominant terms}) \tag{6}$$

where α is the real part of the pole of the Dirichlet series,

$$D(s) \equiv \sum_{n=1}^{\infty} \frac{a_n}{n^s}, \tag{7}$$

and κ is given by

$$\kappa = \frac{D(0) - 1 - \alpha/2}{1+\alpha}. \tag{8}$$

Explicit forms of A and B which we have omitted in the above are also given by the Meinardus's theorem. For the Type I models, we have $\alpha = 1$ and $\kappa = -3/4$:

$$p(n) = \mathrm{const}\, n^{-3/4}\exp(B\sqrt{n}), \tag{9}$$

where $B = \pi/\sqrt{3}$. [11] For the Type II models, a related theorem (Ref. [11], page 99-100, example 10 and 11) assures the same asymptotic form (9) with $B = \pi/\sqrt{6}$. It is also possible to relate Type II models with the Meinardus's theorem (Chap.1 and 6 in ref. [11]). We thus have derived the exact asymptotic form of $p(n)$.

Using (4) and changing the summation into the integration, we finally obtain

$$m \sim n^{-1/4}\exp(B\sqrt{n}), \tag{10}$$

for the Type I and II models. How well the DMRG calculation for the $S = 1/2$ XXZ chain reproduces the asymptotic behavior (10) is demonstrated in Fig.1. In the actual calculation, we have employed the quantum version of the PWFRG, [12–14] by which we obtain the fixed-point wavefunction of the DMRG efficiently.

We give a comment on the universality of the asymptotic form (10) among the integrable systems. In the case where $\{a_n\}$ forms a periodic series or the model itself admits a direct partition-theoretic interpretation, [15,16] the $\exp(B\sqrt{n})$-behavior is universal (Ref. [11], Chapter 6, examples 1-16). The exponent κ may, however, have possibility of model-dependence (due to $D(0)$), modifying the prefactor $n^{-1/4}$ in (10).

Let us now proceed to non-integrable cases, where the exact diagonal form of the CTM or the DM is not known. The DM eigenvalue is no longer given by z^{integer} with single parameter z, or equivalently, log(DM eigenvalue) has not equal-spacing distribution. Both the integer n characterizing the DM eigenvalue, and the quantity $p(n)$ which is essential in the integrable cases lose meaning. Our first task is, then, to translate the result of integrable cases into the one which has meaning also for non-integrable cases.

Writing the m-th DM eigenvalue (including degeneracy) as ω_m, we have $n = \log\omega_m/\log z$ in the integrable case. Substituting $n = \log\omega_m/\log z$ into (10), we have

$$m \sim \left(\frac{\log\omega_m}{\log z}\right)^{-1/4}\exp\left(B\sqrt{\frac{\log\omega_m}{\log z}}\right), \tag{11}$$

or equivalently,

$$\log\left[m\left(\frac{\log\omega_m}{\log z}\right)^{1/4}\right] = B\sqrt{\frac{\log\omega_m}{\log z}}. \tag{12}$$

From (12), we obtain the leading asymptotic form

$$\omega_m \sim \exp[-\text{const.}\ (\log m)^2], \tag{13}$$

where const. $= |\log z|/B^2$ for the integrable cases. Clearly, expressions (11)-(13) do not contain the parameter n which is specific to the integrable models.

There arises an intriguing conjecture: the asymptotic forms (11)-(13) would also apply to non-integrable systems with B and z being suitably redefined. In the "neighborhood" of an integrable model with small non-integrable perturbations added, we may well expect this conjecture to be true: In spite of the non-integrable perturbations, the "stairway structure" (or degeneracy) in the DM eigenvalue spectrum still remains in somewhat smeared-out way, leaving the "envelope" of the ω_m-m curve essentially unchanged. As a check of the universality for the nearly-integrable cases, we made the CTMRG calculations for two systems: the square-lattice Ising model at the critical temperature in finite external field and the 3-states Potts model slightly below the critical temperature (see Fig.2 and Fig.3). We see clear agreements between the CTMRG calculations and the "universal asymptotic form".

As a test of the universality of (11)-(13) for systems far from the integrability, we take the $S = 1$ antiferromagnetic Heisenberg spin chain. For calculation of the DM eigenvalue spectrum, we employ the quantum version of the PWFRG. [12,13] The results are given in Fig.4, which support the universal asymptotic form.

We have made similar calculation for the $S = 1$ bilinear-biquadratic spin chain at $\beta = -0.5$ with the Hamiltonian $\mathcal{H} = \sum \vec{S}_i \cdot \vec{S}_{i+1} + \beta \sum (\vec{S}_i \cdot \vec{S}_{i+1})^2$, whose result (not shown in this Letter) also supports the universality of the asymptotic form.

To summarize, we have discussed the asymptotic distribution of the density-matrix (DM) eigenvalues for non-critical systems (one-dimensional quantum and two-dimensional classical), which controls the accuracy of the density-matrix renormalization group. Based on the equivalence between the DM and the corner transfer matrix (CTM), we derived the exact asymptotic form of the DM eigenvalue distribution for a class of integrable models. The resulting expression has been rewritten in a "universal" form which does not contain quantities specific to integrable models. Numerical-renormalization-group calculations using the CTMRG and the product-wavefunction RG have been performed for non-integrable models, which shows that the non-integrable models actually have the same asymptotic form of the DM-eigenvalue distribution, in strong support of the universality of the asymptotic form.

There remains many important problems left for future studies. A more "physical" explanation to justify the universal asymptotic form is desired. How universal the obtained asymptotic form, itself remains to be a question to be answered; there may well be different "universal classes" of the DM. In fact, the valence-bond-solid (VBS) models [17], have only finite-dimensional DMs which sharply contrast to the ones studied in this Letter. Relation between the DM-eigenvalue distribution and the finite-m (m: number of retained bases) behavior of physical (observable) quantities has not been known, although there have been a few works discussing the "finite-m scaling"(2D classical [18], transverse-field XXZ chain [19]). Behavior of the DM for critical system is also an important subject of study. [20,21] Our study made in the present Letter may be a first step for clarification of these problems. [22]

This work was partially supported by the Grant-in-Aid for Scientific Research from Ministry of Education, Science, Sports and Culture (No.09640462), and by the "Research for the Future" program of the Japan Society for the Promotion of Science (JSPS-RFTF97P00201). One of the authors (K. O.) is supported by JSPS fellowship for young scientists, and (Y. H.) is partly supported by the Sasakawa Scientific Research Grant from The Japan Science Society.

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[1] S.R. White, Phys. Rev. Lett. **69**, 2863 (1992); Phys. Rev. **B 48**, 10345 (1993).

[2] S.R. White and D.A. Huse, Phys. Rev. B **48**, 3844 (1993); S. R. White, to appear in Phys. Rep.. See also G.A. Gehring, R.J. Bursill and T. Xiang, Acta Phys. Pol. A **91**, 105 and references cited therein. (1997).

[3] T. Nishino, J. Phys. Soc. Jpn. **64**, 3598 (1995).

[4] T. Nishino and K. Okunishi, J. Phys. Soc. Jpn **67**, 3066 (1998).

[5] T. Nishino and K. Okunishi, J. Phys. Soc. Jpn.**65**, 891 (1996); J. Phys. Soc. Jpn. **66**, 3040 (1997).

[6] T. Nishino and K. Okunishi, J. Phys. Soc. Jpn. **64**, 4084 (1995).

[7] R.J. Baxter, J. Math. Phys. **9**, 650 (1968); J. Stat. Phys. **19**, 461 (1978).

[8] R.J. Baxter, J. Stat. Phys. **15**, 485 (1976); J. Stat. Phys. **17**, 1 (1977).

[9] R.J. Baxter "Exactly Solved Models in Statistical Mechanics" (1982) Accademic Press.

[10] S.Östlund and S.Rommer, Phys. Rev. Lett **75**, 3537 (1995); Phys. Rev. B **55**, 2164 (1997).

[11] G.E. Andrews, "The Theory of Partitions"(1976) Addison-Wesley, Reading, Massachusetts.

[12] Y. Hieida, K. Okunishi and Y. Akutsu, Phys. Lett. A **233**, 464 (1997).

[13] K. Okunishi, Y. Hieida amd Y. Akutsu, cond-mat/9807266.

[14] R. Sato and Y. Akutsu, J. Phys. Soc. Jpn **65**, 1885

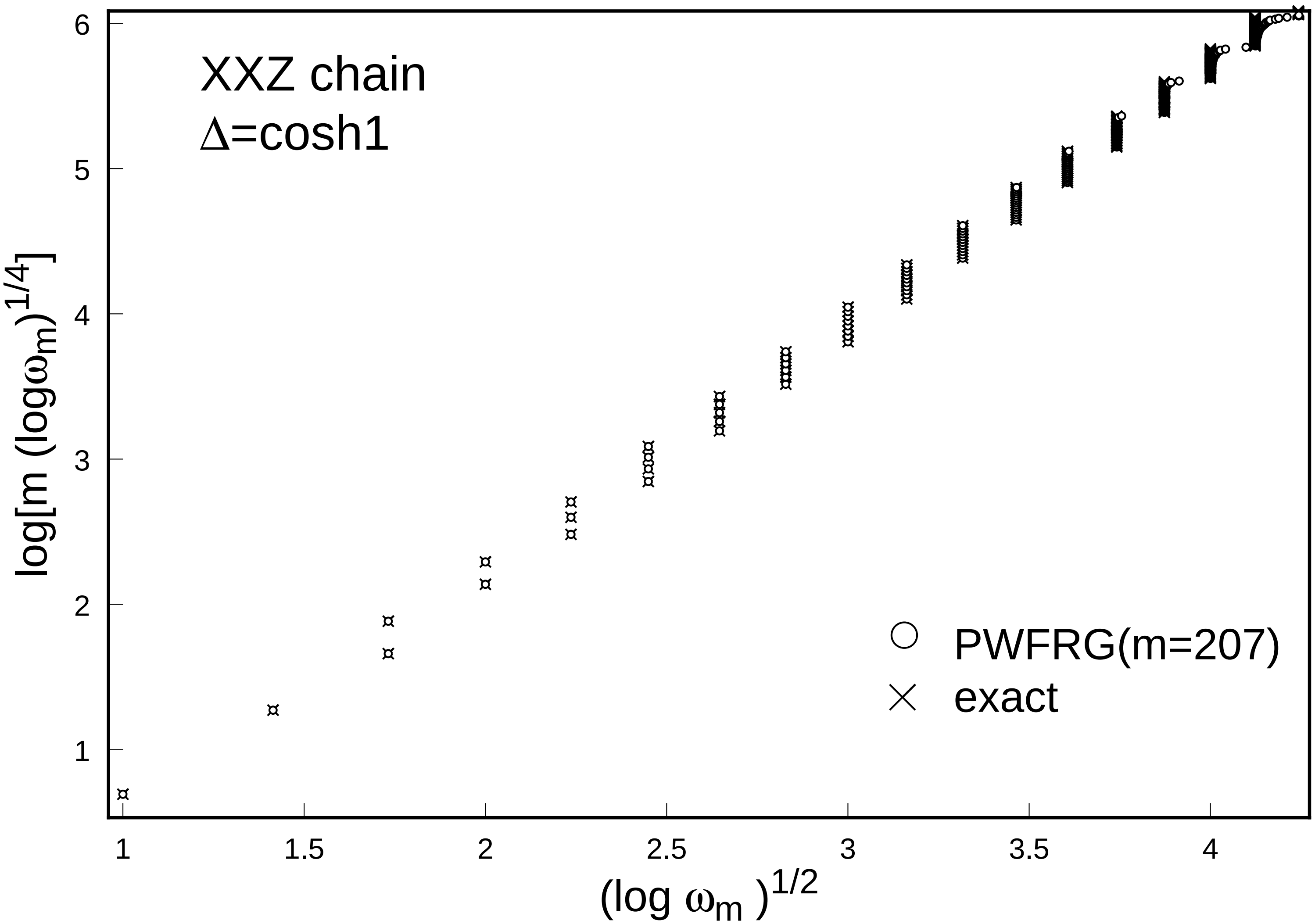
(1996).
[15] R.J. Baxter and P.A. Pearce, J. Phys. A: Math. Gen. **15**, 897 (1982); J. Phys. A: Math. Gen. **16**, 2239 (1983).
[16] G.E. Andrews, R.J. Baxter and P. Forrester, J. Stat. Phys. **35**, 193 (1984).
[17] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Phys. Rev. Lett. **59**, 799 (1987); Commun. Math. Phys. **115**, 477 (1988).
[18] T. Nishino, K. Okunishi and M. Kikuchi, Phys. Lett. A **213**, 69 (1996).
[19] Y. Hieida, unpublished.
[20] M. Andersson, M. Boman and S. Ostlund, cond-mat/9810093.
[21] T.T. Troung and I. Peschel, Z. Phys. B **69**, 385 (1987); **75**, 119 (1988); B. Davies and P. Pearce, J. Phys. A: Math. Gen. **23**, 1295 (1990).
[22] After completion of the present work, a preprint verifying the relation DM = CTM^4 (asymptotic behavior is not discussed) for the transverse-field Ising chain appears: I. Peschel, M. Kaulke and Ö. Legeza, cond-mat/9810174.

FIG. 1. PWFRG calculation of density-matrix eigenvalues $\{\omega_m\}$ for $S = 1/2$ antiferromagnetic XXZ chain and comparison with the exact spectrum. We take the exchange coupling constants to be $|J_x| = |J_y| = 1$ and $|J_z| = \Delta = \cosh(1)$. Number of retained bases in the PWFRG calculation is $m = 207$.

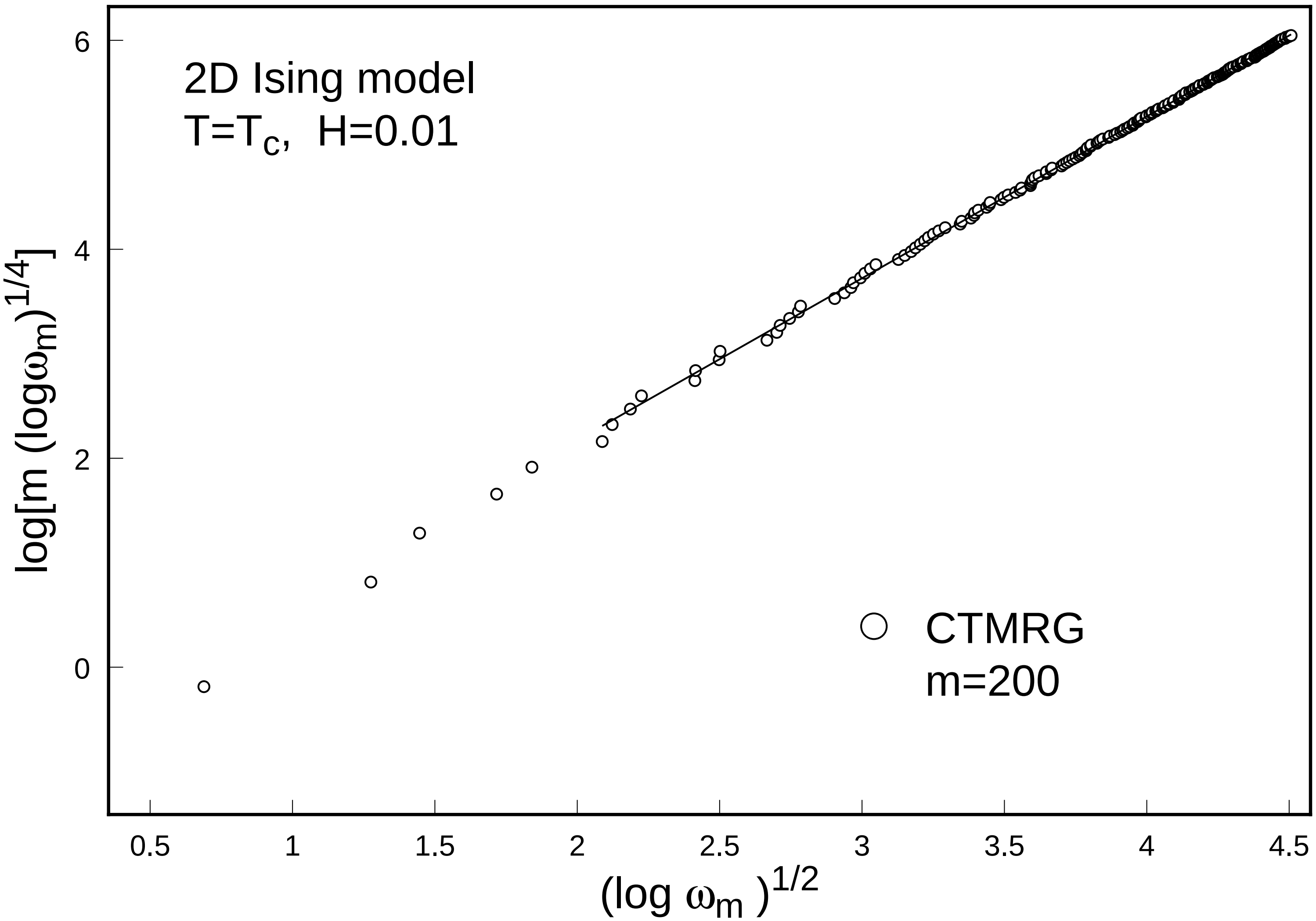
FIG. 2. CTMRG calculation ($m = 200$) of the density-matrix eigenvalues $\{\omega_m\}$ for the square-lattice Ising model at a critical temperatur T_c in a small external field H. We have also drawn a line corresponding to the universal asymptotic form.

FIG. 3. CTMRG calculation ($m = 242$) of the density-matrix eigenvalues $\{\omega_m\}$ for the 3-state Potts model slightly below the critical temperature. We have also drawn a line corresponding to the universal asymptotic form.

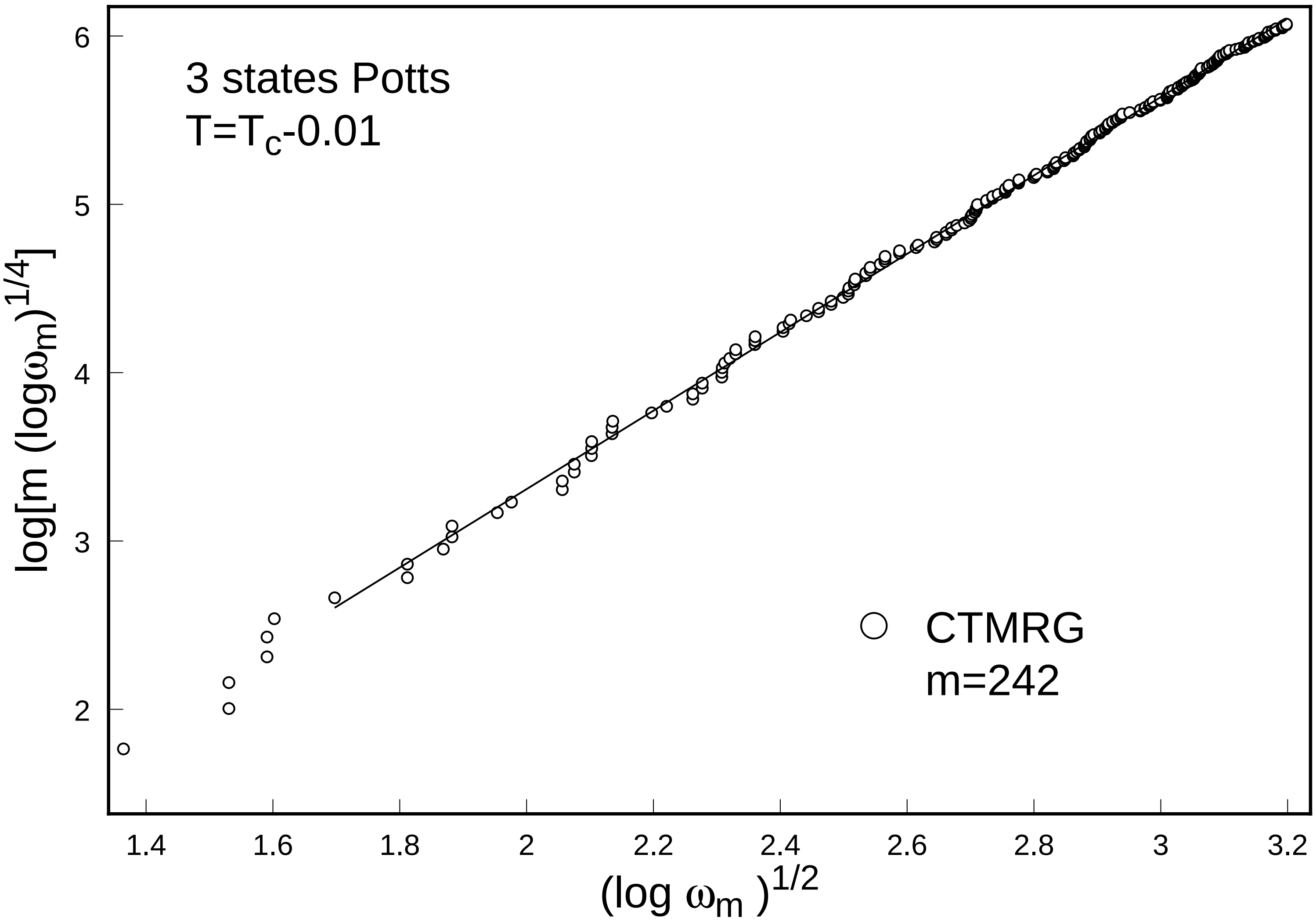
FIG. 4. PWFRG calculation ($m = 700$) of density-matrix eigenvalues $\{\omega_m\}$ for $S = 1$ antiferromagnetic Heisenberg chain. We have also drawn a line corresponding to the universal asymptotic form.



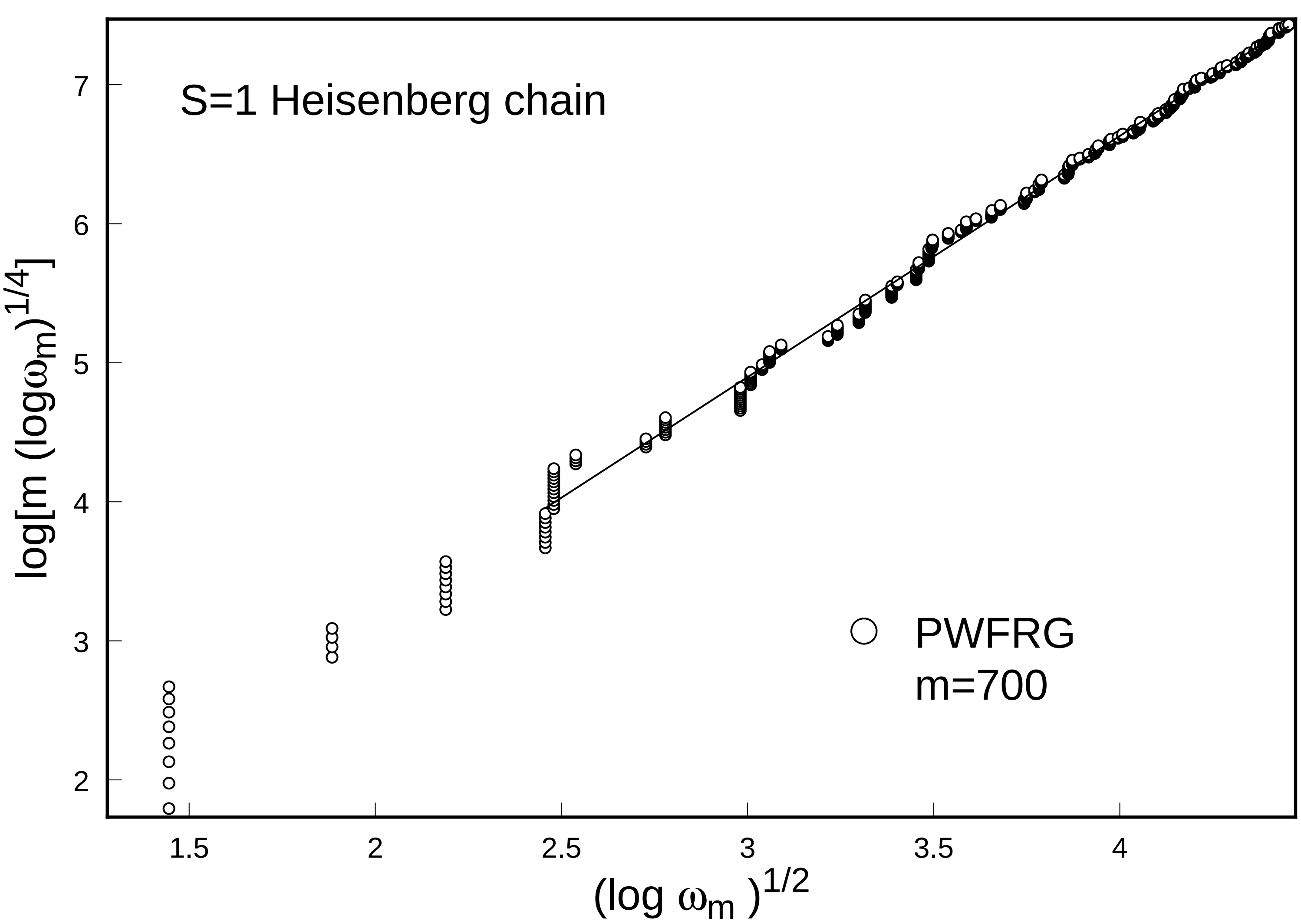
K. Okunishi, Y. Hieida and Y. Akutsu Fig.1



K. Okunishi, Y. Hieida and Y. Akutsu Fig.2



K. Okunishi Y. Hieida and Y. Akutsu Fig.3



K. Okunishi Y. Hieida and Y. Akutsu Fig.4